Nuclear Density-Functional theory: achievements and open ends

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Outline

1. Ingredients: nuclear DFT, empirical calibration, observables
2. Achievements: energies and charge formfactors
3. Open ends: homework problems and perspectives
4. Conclusions

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1) Ingredients: nuclear DFT, empirical calibration, observables

Nuclar DFT models (zero range, non-relativistic)

variational formulation on the basis of a given energy functional (time even part only)

$$E_{\rm tot} = E_{\rm kin} + \int d^3r\, \mathcal{E}_{\rm model}(\rho_0, \rho_1, \tau_0, \tau_1, \mathbf{J}_0, \mathbf{J}_1, \tilde{\rho}_p, \tilde{\rho}_n) + E_{\rm Coulomb} - E_{\rm c.m.} - E_{\rm rot} - E_{\rm corr}$$

- $\tilde{\rho}_p, \tilde{\rho}_n$ → pairing density
- $\mathbf{J}_0, \mathbf{J}_1$ → spin-orbit density
- τ_0, τ_1 → kinetic density
- ρ_0, ρ_1 → density, $\rho_{0/1} = \rho_n \pm \rho_p$

$\mathcal{E}_{\rm model} = C_0^{(\rho)}\, \rho_0 * \rho_0$	$+C_1^{(\rho)}\, \rho_1 * \rho_1$	volume	$C_{0,1}^{(\rho)}$ dens.dep.
$+C_0^{(\nabla)}\, \nabla\rho_0 * \nabla\rho_0$	$+C_1^{(\nabla)}\, \nabla\rho_1 * \nabla\rho_1$	surface	$C_0^{(\nabla)} = C_0^{(\nabla)}(\nabla\rho_0)$
$+C_0^{(\tau)}\, \rho_0 * \tau_0$	$+C_1^{(\tau)}\, \rho_1 * \tau_1$	kinetic	
$+C_0^{(ls)}\, \rho_0 * \nabla\mathbf{J}_0$	$+C_1^{(ls)}\, \rho_1 * \nabla\mathbf{J}_1$	spin orbit	
$+C_p^{(\rm pair)}\, \tilde{\rho}_p * \tilde{\rho}_p$	$+C_n^{(\rm pair)}\, \tilde{\rho}_n * \tilde{\rho}_n$	pairing	

$$C_t^{(\rm pair)} = C_{t,0}^{(\rm pair)} + C_{t,1}^{(\rm pair)}\rho_0 + \underbrace{C_{t,\nabla}^{(\rm pair)}(\nabla\rho_0)^2}_{\text{Fayans}}$$

relativistic mean-field (RMF): zero range $\equiv$ point coupling $\rightarrow$ RMF-PC
finite range $\rightarrow$ dens.dep. meson coupling RMF-DD

$\Longrightarrow$: typically 11–15 model parameters $\leftrightarrow$ tuned to empirical data $\hookrightarrow$

Strategy for adjusting the model parameters to phenomenological data

theoretical model:
parameters $\boldsymbol{\theta} = (\theta_1 \ldots \theta_{N_p})$
$\Rightarrow$ observables $y^{(\mathrm{th})}(\boldsymbol{\theta})$

pool of fit data:
$\mathbf{y}^{(\mathrm{exp})} = (y_1^{(\mathrm{exp})} \ldots y_{n_d}^{(\mathrm{exp})})$

objective function:

$$\chi^2(\boldsymbol{\theta}) = \sum_{d \in \{\mathrm{data}\}} \frac{(y_d^{(\mathrm{th})}(\boldsymbol{\theta}) - y_d^{(\mathrm{exp})})^2}{\delta y_d^2}$$

minimal χ^2: best fit $\boldsymbol{\theta}_0$ $\longrightarrow$ predictions $y_n^{(\mathrm{th})}(\boldsymbol{\theta}_0)$

vicinity $\boldsymbol{\theta}_0$: statistical interpretation $p(\boldsymbol{\theta}) \propto e^{-\chi^2(\boldsymbol{\theta})} \equiv$ probability distribution
$\Rightarrow$ variances ($\equiv$ from leeway of model parameters)
covariances $\equiv$ Coeff. of Determination (CoD) , sensitivity analysis

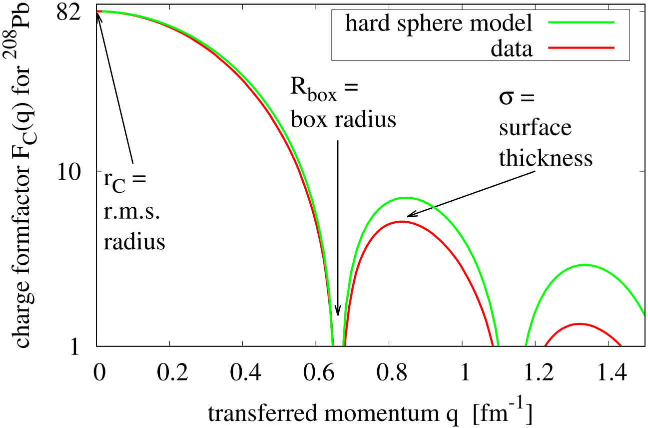
error propagation: from residuals of E_B, r_C, ... using Bayesian calculus
$\longrightarrow$ typically factor 2 larger than from statistical analysis

Observables from charge density $\rho_C(r)$ & formfactor $F(q)$

Muonic atoms: quality source for Barrett radius $\langle r^k e^{-\alpha r}\rangle \xrightarrow{\text{model}}$ rms radius r_C

Optical methods: high precision for isotopic r_C^2 differences (soon also: r_C^4)

Charge formfactor from electron scattering:



low q ($< 2/\text{fm}$)
free from correlations
$\Longrightarrow$ safe in DFT

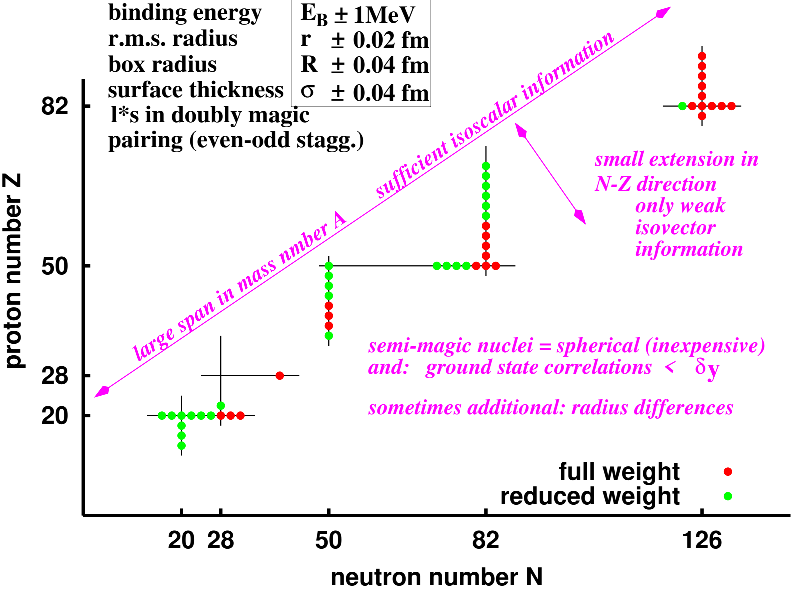
$\Longrightarrow$ **form parameters**
r_C, R_{box}, σ_C, halo

involved exp. analysis
$\Longrightarrow$
robust for stable nucl.
unsafe isotopic diff.
no exotic nuclei yet

$$F_C = \sum_{t=p,n} \left(F_t * g_t + F_{ls,t} * g_{\mathrm{mag},t}\right) \ , \ g = \text{nucleon intrinsic formf.}, F \text{ from mean field calc.}$$

"Standard" fit data – ground state properties (Klüpfel et al, PRC **79** (2009) 034310)

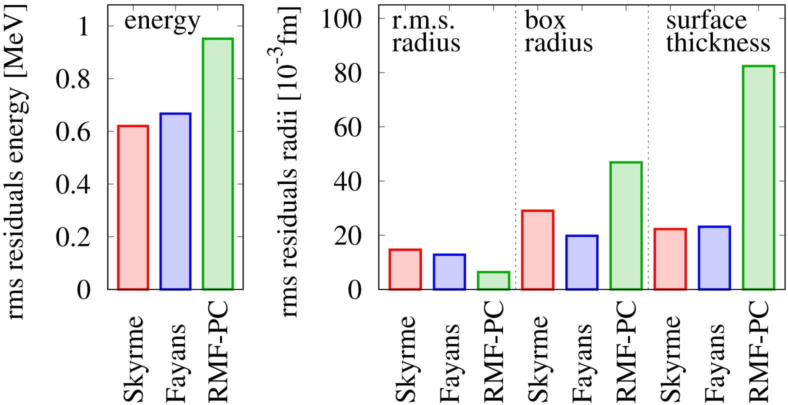
Fit Observables:	y	δy
binding energy	E_B	$\pm$ 1MeV
r.m.s. radius	r	$\pm$ 0.02 fm
box radius	R	$\pm$ 0.04 fm
surface thickness	σ	$\pm$ 0.04 fm
l*s in doubly magic		
pairing (even-odd stagg.)		



2) Achievements: energies and charge formfactors

Global quality of DFT fits (in terms of rms residuals)

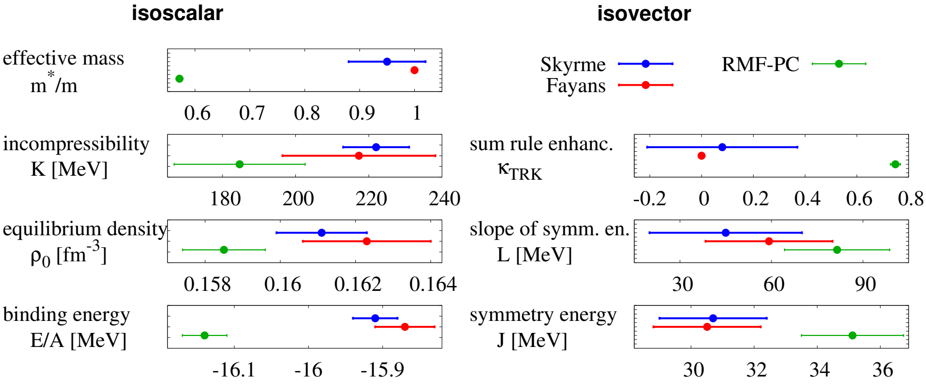
3 different DFT functionals: Skyrme & Fayans, relativistic point-coupling (RMF-PC)
all fitted to the same “standard” data



comparable (high) quality of nuclear bulk prop. - in spite of different density dependence

RMF-PC less flexible in describing formfactor parameters (reason ???)

Extrapolation to symmetric nuclear matter properties (NMP)



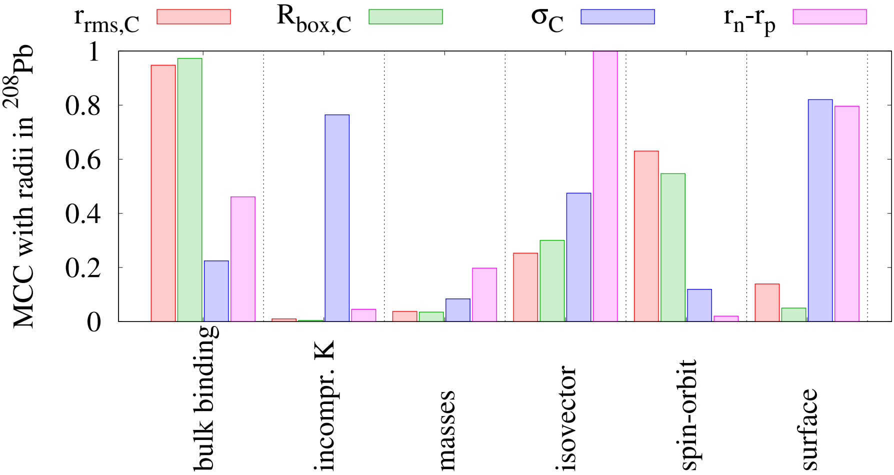
the two non-relativistic models (Skyrme & Fayans) make similar predictions

the relativistic RMF-PC model predicts substantially different NMP

$\longleftrightarrow$ effective masses m^*/m and κ_{TRK} make the major difference

RMF $\leftrightarrow$ non-relativistic: similar for stable nuclei, different for super-heavy elements

Multiple Correlation Coefficients (MCC) with radii in ^{208}Pb



$r_{rms,C}$&$R_{\rm box}$ very similar $\leftrightarrow$ mostly bulk binding, some I$*$s, also some pairing

σ_C $\leftrightarrow$ incompressibility K & surface, some isovector (symmetry energy)

neutron skin $r_{rms,n} - r_{rms,p}$ $\leftrightarrow$ 99% isovector, also some surface

note: for Skyrme fit without radius information ($r_{rms,C}$, $R_{box,C}$, σ_C)!

Information from differences of bulk observables

Differences of observables yield new information, other than the observables as such:

energy difference:

separation energy $\leftrightarrow$ Fermi energy.

3. energy difference (odd-even energy staggering):

$\Delta_p^{(3)} \leftrightarrow$ proton pairing, $\Delta_n^{(3)} \leftrightarrow$ neutron pairing.

neutron-proton radius difference (skin):

explores predominantly symmetry energy ($\hookrightarrow$)

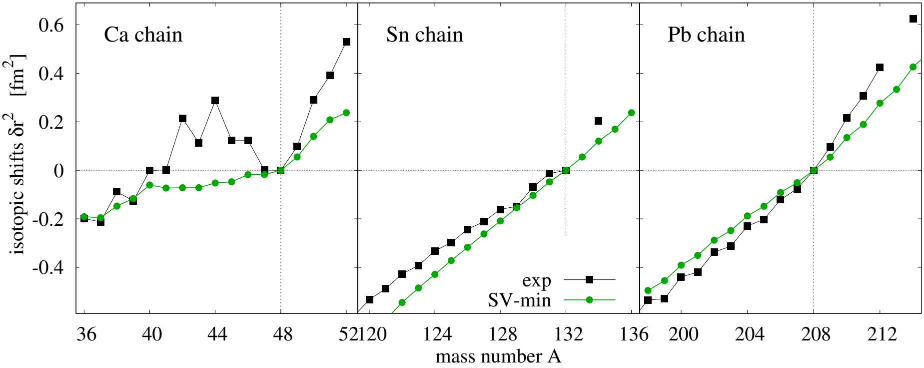
isotopic radius difference:

pairing, spin-orbit, surface structure (depending on nucleus) $\hookrightarrow$

radius odd-even staggering:

pairing surface energy $\hookrightarrow$

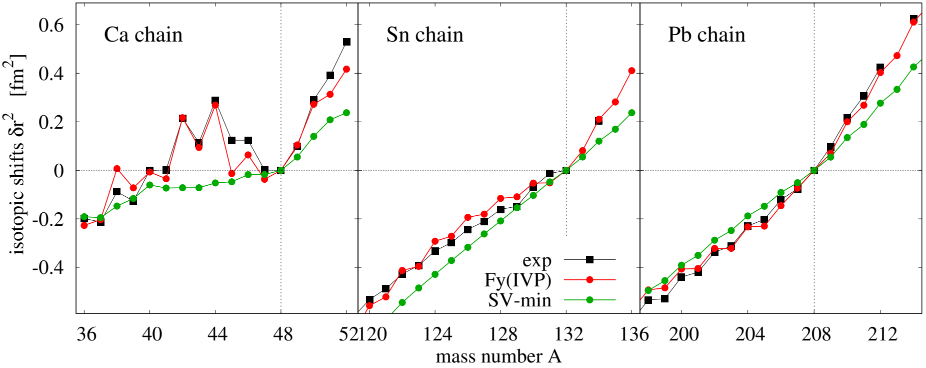
Radius differences: isotopic trend δr_C^2 and odd-even staggering



fit to bulk data (Skyrme SV-min) fails in predicting isotopic trends of radii

fit of Skyrme functional to δr_C extended data $\Longrightarrow$ impossible to meet the trends

Radius differences: isotopic trend δr_C^2 and odd-even staggering



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fit of Skyrme functional to δr_C extended data $\Longrightarrow$ impossible to meet the trends

Fayans: gradient in pairing $\propto \tilde{\rho}^2(\nabla\rho_0)^2$ & in surface term $\Longrightarrow$ trends well reproduced

$\Longrightarrow$ new data force extension of the functional and help model development

3) Open ends: homework problems and perspectives

3) Open ends: problems and promising perspectives

Neutron radius r_n:

from A_{PV} (CREX/PREX)& polarizability $\alpha_D \Rightarrow$ conflicting data

Binding energies E_B of super-heavy elements:

Skyrme under-estimates $E_B \leftrightarrow$ RMF over-estimates E_B,
but energy differences ($S_{2n/2p}$, Q_α) well predicted

Giant dipole resonance (GDR):

E_{GDR} in heavy nuclei o.k., but trend $E_{GDR}(Z, N)$ toward light nuclei wrong.

Low-lying collective modes, fission:

Large span of predictions $\longrightarrow$ use data for model development? (pairing)

Structure of functionals:

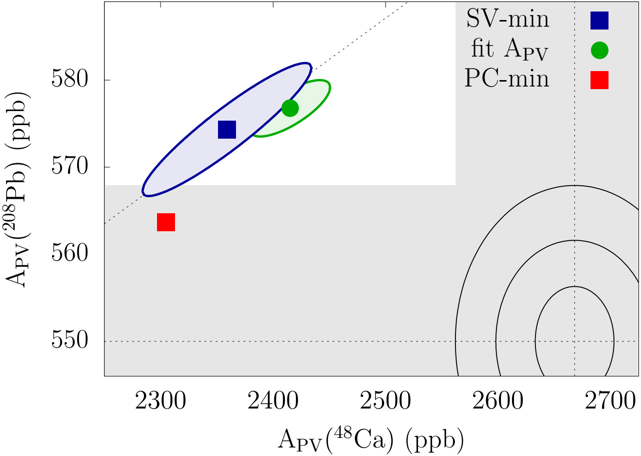
finite-range attractive term from explicit pion-exchange
$\Rightarrow$ degrades surface thickness σ_C

Fourth moment of charge radius $r_{C,4}$:

Quality data expected soon $\longleftrightarrow$ $r_{C,4}$ highly correlated with σ_C
$\Rightarrow$ surface thickness for unstable elements.

Compatibility of A_{PV} measurements in ^{208}Pb and ^{48}Ca

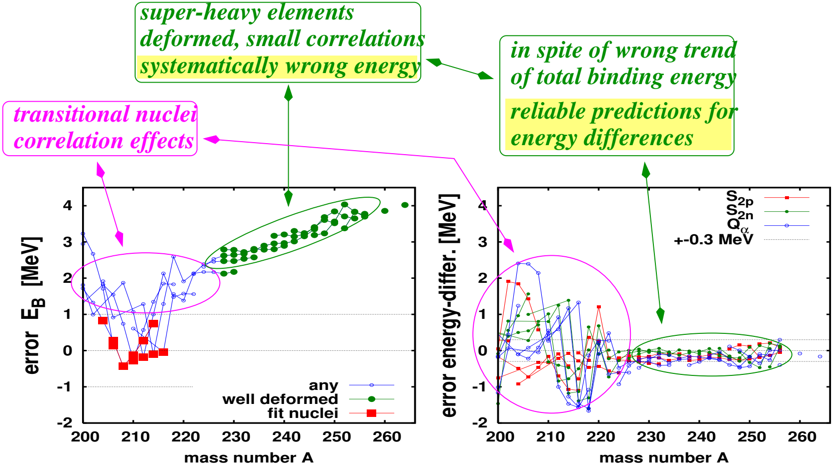
A_{PV} = parity violating asymmetry, from high-E polarized electron scattering



error ellipsoids (limits of the model) avoid the goal
attempt to fit additionally both A_{PV} does not work

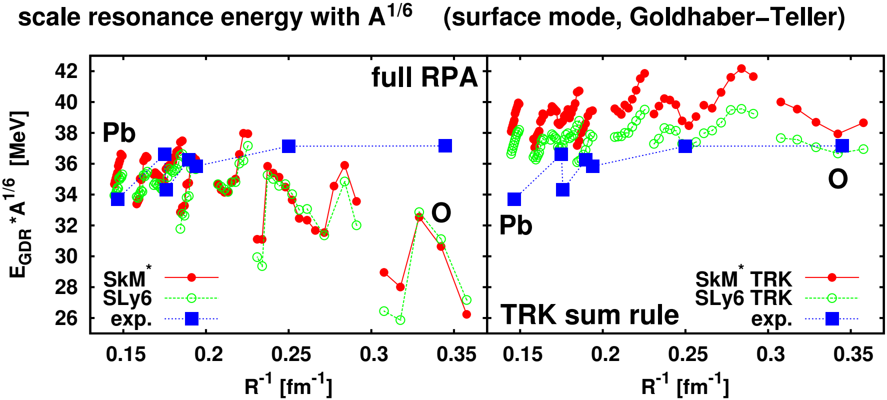
Extrapolations to super-heavy elements

binding energy: E_B & energy differences: S_{2n} , S_{2p}, Q_α



DFT remains useful for describing superheavy elements

Problem with reproducing trends of GDR with *A*

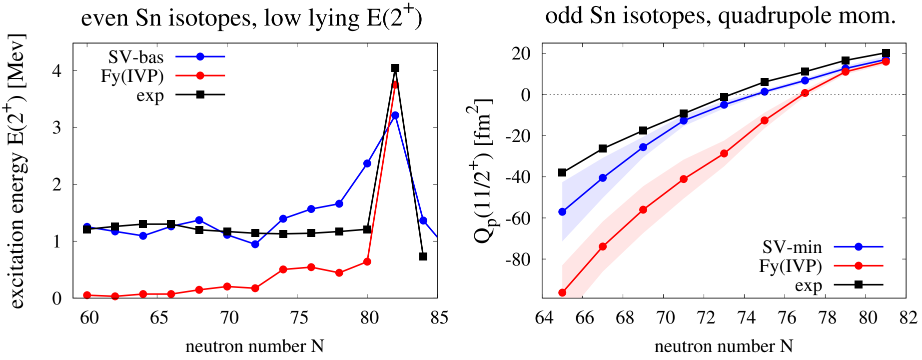


experiment follows nicely $A^{1/6}$ trend

RPA result tend to $A^{1/3}$ (volume mode)

TRK mode follows also $A^{1/6}$ trend

Next steps in Fayans model development

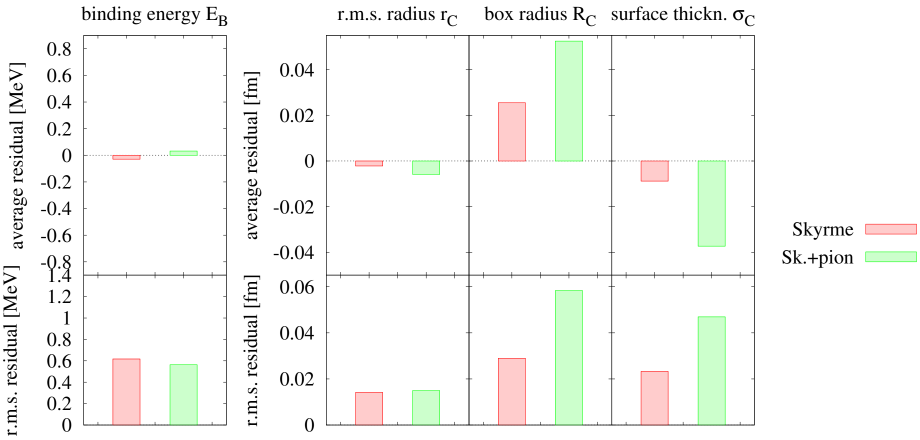


pairing signatures: low lying $E(2^+)$ energies $\longleftrightarrow$ too low
quadrupole moments Q_p $\longleftrightarrow$ too large

$\Longrightarrow$ Fy(IVP) has too weak neutron pairing
$\Longrightarrow$ need more $p \leftrightarrow n$ pairing terms, enough δr^2 data for relevant fit

Finite-range functionals (long-range pion contribution from chiral $\mathcal{L}$)

add pion-term to Skyrme DFT, readjust Skyrme parameters (coop. L. Zurek, A. Schwenk)



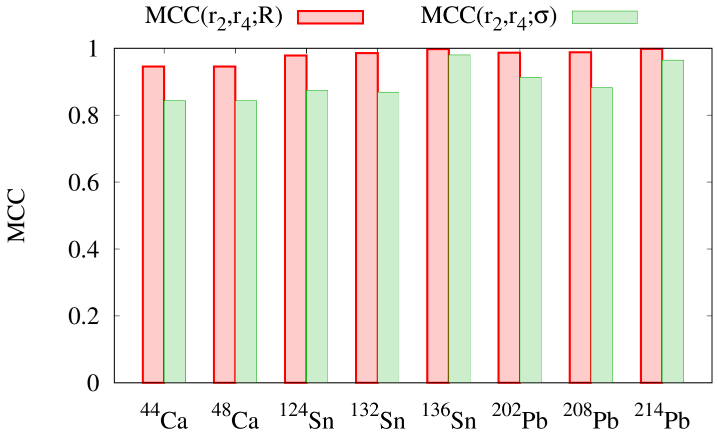
Skyrme ↔ Sk.+pion: equivalent for E_B & r_C, pion unfriendly to R_C & σ_C

happens for any finite-range attractive term, resolved by adding finite-range repulsive term

Fourth moment of charge radius $r_{C,4} \longleftrightarrow \sigma_C$

Optical measurement + elaborate analysis $\Longrightarrow$ determine also $r_4 = (\langle r_C^4 \rangle / Z)^{1/4}$

Can r_C&$r_{C,4}$ predict σ_C? $\longrightarrow$ multiple correlation analysis



r.m.s. radius r_2 together with r_4 approx. equivalent to information from R and σ

$\Longrightarrow$ more data on nuclear formfactor for exotic nuclei, precision should be < 0.01 fm

Conclusions

Nuclear DFT, calibration & statistical interpretation:

energy-density functionals $\longrightarrow$ description of energies and densities
structure motivated by low-q expansion, parameters tuned to empirical data
χ^2 fit & statistical analysis $\longrightarrow$ predictions with error bands, correlations

Form parameters:

density $\longrightarrow$ formfactor $\longrightarrow r_{rms}, R_{box}, \sigma$
charge formfactor $F_C(q) \longleftarrow F_p(q), F_n(q), F_{ls,p}(q), F_{ls,n}(q)$& nucleon formf.

Performance:

high quality bulk properties ($E_B, r_{\mathrm{rms,C}}, R_{\mathrm{box,C}}, \sigma_C$) from ^{16}O to actinides
radius differences $\delta r_C^2 \leftrightarrow$ require Fayans functional ($(\nabla\rho)^2$ in E_{pair}&E_{surf})
neutron skin $\leftrightarrow$ symmetry energy J, L

Future development:

neutron radius (PREX/CREX),E_B in super-heavy elements, trend of GDR
use info from low-lying collective modes, fission ($\leftrightarrow$ pairing)
use info info from ab-initio models (finite range, density dependence, pairing)
upcoming information on $\langle r_C^4\rangle \longleftrightarrow \sigma_C$, $\delta\sigma_C$ in exotic nuclei